Butanoic acid, propyl ester
105-66-8 DTXSID6059318

Model Performance

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 147 °C

Global applicability domain: Inside

Local applicability domain index: 1.00

Confidence level: 9.41e-01

Nearest Neighbors from the Training Set

Image not found

Butanoic acid, propyl ester

Measured: 143 Predicted: 147 Image not found

Ethyl valerate

Measured: 146 Predicted: 147 Image not found

Butyl propionate

Measured: 147 Predicted: 147

Image not found

Pentyl acetate Measured: 149 Predicted: 147 Image not found

Methyl hexanoate
Measured: 150
Predicted: 147